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Donald E. Williams
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This report describes a computer program which refines lattice constants for any crystal symmetry by the least squares method. Several types of extrapolation functions are provided, and these functions can be used either singly or in combination. A complete error treatment is made, including covariances between parameters.

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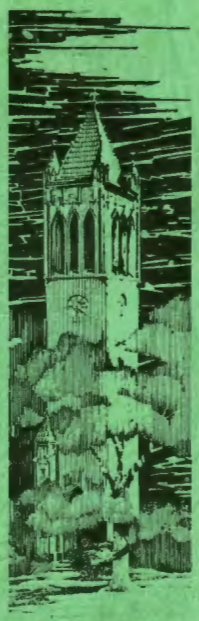

IOWA STATE UNIVERSITY

LCR-2, A FORTRAN LATTICE CONSTANT REFINEMENT PROGRAM

by

Donald E. Williams

AMES LABORATORY

RESEARCH AND DEVELOPMENT REPORT

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LCR-2, A FORTRAN LATTICE CONSTANT REFINEMENT PROGRAM

by

Donald E. Williams

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ABSTRACT

This report describes a computer program which refines lattice constants for any crystal symmetry by the least squares method. Several types of extrapolation functions are provided, and these functions can be used either singly or in combination. A complete error treatment is made, including covariances between parameters.

MATHEMATICAL METHOD

A residual function, R, of the parameters, p_k, is defined by the equation $R = \Sigma w \left[\Delta(p_k)\right]^2$. This function is minimized by expanding the residuals $\Delta(p_k)$ in a first order Taylor's series about the trial values, setting the partial derivatives of R equal to zero, and solving the resulting set of linear equations for the parameter corrections ϵ_k. The summation is over the observed reflection data, and the weighting factors w are defined by $w = 1/\sigma^2(\Delta)$, where $\sigma(\Delta)$ is the estimated standard deviation of Δ. The linear equations may be written in matrix notation as $\underset{\sim}{C}\,\underset{\sim}{\epsilon} = \underset{\sim}{q}$, where

$$C_{ij} = \Sigma w \frac{\partial \Delta}{\partial p_i} \frac{\partial \Delta}{\partial p_j} \quad \text{and} \quad q_i = \Sigma - w \Delta \frac{\partial \Delta}{\partial p_i} \quad .$$

The parameter list defined by this program is the following: the first three parameters are the lengths of the unit cell edges in Å, the second three parameters are the cell angles in degrees, and the last

four parameters are extrapolation function coefficients, to be defined later. Any combination of these ten parameters may be refined by the program.

The residual Δ is defined by the equation

$$\Delta = (d^*)^2 - 4 \sin^2\theta/\lambda^2 - 4 \Delta\theta \sin 2\theta/\lambda^2 \ ,$$

$$\Delta\theta = \sum_n^4 K_n f_n(\theta) \ .$$

Thus the systematic error in θ, $\Delta\theta$, is expressed as the sum of contributions from various sources having the functional form $f_n(\theta)$ and coefficient K_n.

We now must find expressions for the various derivatives of d^*. The quantity d^* may easily be expressed as a function of the reciprocal lattice constants; however, since we have chosen to refine the direct constants, we must express d^* and its derivatives as functions of the direct lattice constants. In terms of the metric tensor $\underset{\sim}{g}$, where

$$\underset{\sim}{g} = \begin{pmatrix} p_1p_1 & p_1p_2\cos p_6 & p_1p_3\cos p_5 \\ p_1p_2\cos p_6 & p_2p_2 & p_2p_3\cos p_4 \\ p_1p_3\cos p_5 & p_2p_3\cos p_4 & p_3p_3 \end{pmatrix} \ , \quad (d^*)^2 = \underset{\sim}{h}\, \underset{\sim}{g}^{-1}\, \underset{\sim}{h}, \text{ where}$$

$\underset{\sim}{h}$ is the vector of the Miller indices of the reflection.

Although the expressions for the derivatives of $\underset{\sim}{g}^{-1}$ with respect to the p_k may be obtained in closed form, they are rather lengthy. This program evaluates these derivatives numerically by incrementing the p_k. The increments chosen are 0.005 Å for the cell edges, and 0.5° for the cell angles. The derivatives of $\underset{\sim}{g}^{-1}$ need be calculated only once,

since $\frac{\partial (d^*)^2}{\partial p_k} = \sum_i^3 \sum_j^3 h_i h_j \frac{\partial g_{ij}^{-1}}{\partial p_k}$. Thus a table may be constructed with the 54 derivatives of each of the elements of $\underset{\sim}{g}^{-1}$ with respect to p_k. Since $\underset{\sim}{g}^{-1}$ is symmetric, only 36 of these are independent.

The derivatives of Δ with respect to the extrapolation coefficients K_n are simply the extrapolation functions $f_n(\theta)$, multiplied by $4 \sin 2\theta/\lambda^2$.

EXTRAPOLATION FUNCTIONS

A discussion of extrapolation functions suitable for typical experimental arrangements is given in the International Tables for X-Ray Crystallography, Vol. II, p. 216 (1959). References to the extensive literature on this subject may also be found there.

Program LCR-2 provides a choice of any combination of the four extrapolation functions listed below. The user may alter the program, if necessary, to change these functions to suit his preference or experimental method.

1. $\Delta\theta_1 = K_1 \sin 2\theta$. This is equivalent to a linear extrapolation of a plot of d vs $\cos^2\theta$ to $\theta = 90°$. This function may be used to correct for eccentricity of the sample.
2. $\Delta\theta_2 = K_2 \cos\theta$. This is equivalent to a linear extrapolation of a plot of d vs $\cos\theta \cot\theta$ to $\theta = 90°$.
3. $\Delta\theta_3 = K_3 \cos\theta\,(1/2 + \sin\theta/2\theta)$. This is equivalent to a linear extrapolation of a plot of d vs $\frac{1}{2}(\cos^2\theta/\sin\theta + \cos^2\theta/\theta)$ to $\theta = 90°$. This is the procedure suggested by Nelson and Riley to correct for absorption errors in the sample.

4. $\Delta\theta_4 = K_4$. This is equivalent to a linear extrapolation of a plot of d vs cot θ to $\theta = 90°$. This function may be used to correct for a constant calibration error persisting at $2\theta = 180°$. Prior calibration of the experimental apparatus is highly desirable. For example, a substance with accurately known lattice constants, such as Al, may be used for calibration.

It should be noted that these extrapolation functions have a similar mathematical form as θ approaches 90°. The lack of orthogonality between these functions will result in a large correlation between the extrapolation coefficients. For this reason, the results obtained with the program when more than one extrapolation coefficient is varied should be cautiously interpreted.

WEIGHTING FACTORS

After correction for the systematic error $\Delta\theta$, it is presumed that only random errors in θ will remain. Assuming the systematic errors are small, the random error in Δ is given by the equation $\sigma(\Delta) = 8\,\sigma(\theta) \sin\theta \cos\theta/\lambda^2$, and therefore $w = \lambda^4/64\,\sigma(\theta) \sin^2\theta \cos^2\theta$. The effect of these weighting factors on the final values of the parameters is not negligible, and it is therefore important that they be included.

INPUT DATA FORMATS

1. Title card, any alphanumerics in col. 1-70, col. 71-72 blank.
2. Initial lattice constants in angstroms and degrees: FORMAT (6F10.4); a, b, c, alpha, beta, and gamma.

3. Control card. Col. 1-10 have parameter selection information for the six lattice constants and the four extrapolation functions; a 1 in the corresponding column includes the parameter in the least squares treatment, otherwise put zero in the column.

   Col. 20 has the lattice type code. Triclinic=1, monoclinic=2, orthorhombic=3, tetragonal=4, rhombohedral=5, hexagonal=6, or cubic=7.

   Col. 29-30 has the maximum number of least squares cycles desired.

   Col. 31-40, 41-50, and 51-60 have damping factors for the shifts in the magnitudes of the lattice constants, the angular constants, and the extrapolation coefficients. These are normally punched 1.0 unless convergence difficulties are encountered.

   Col. 69-70 has the number of data cards to be considered.

   Control card is FORMAT (10I1, 2I10, 3F10.2, I10).

4. Data cards, FORMAT (6F10.0). These contain h, k, ℓ, two theta, estimated error in two theta, and the wave length.

   Any number of sets of data may be processed without reloading the program. Each data set consists of items 1 to 4 above.

5. Stopper card, any alphanumerics in col. 1-70, 1 in col. 72.

```
      START     ACCNTA0015  @D.WILLIAMS@                                    PCGC
      COMPILE   RUN  FORTRAN LIST                                           PCGC
C      LCR-2  LATTICE CONSTANT REFINEMENT  D.WILLIAMS  APRIL 1964
C      INPUT IS AS FOLLOWS
C      TITLE CARD, FORMAT(14A5,I2)
C      INITIAL LATTICE CONSTANTS IN ANGSTROMS AND DEGREES, FORMAT(6F10.4)
C      CONTROL CARD, FORMAT(10I1,2I10,3F10.2,I10)
C      COL. 1-10 HAS PARAMETER SELECTION INFORMATION FOR THE SIX LATTICE
C        CONSTANTS AND FOUR EXTRAPOLATION FUNCTIONS, 1=SELECT, 0=DO NOT
C        SELECT
C      COL. 11-20 HAS LATTICE TYPE CODE
C        1=TRICLINIC
C        2=MONOCLINIC
C        3=ORTHORHOMBIC
C        4=TETRAGONAL
C        5=RHOMBOHEDRAL
C        6=HEXAGONAL
C        7=CUBIC
C      COL. 21-30 HAS NUMBER OF LEAST SQUARES CYCLES DESIRED
C      COL. 31-40 HAS DAMPING FACTOR FOR TRANSLATIONAL CONSTANT SHIFTS
C      COL. 41-50 HAS DAMPING FACTOR FOR ANGULAR CONSTANT SHIFTS
C      COL. 51-60 HAS DAMPING FACTOR FOR EXTRAPOLATION CONSTANTS
C      COL. 61-70 HAS NUMBER OF DATA CARDS TO BE CONSIDERED
C      DATA CARDS, FORMAT(6F10.0), H, K, L, TWO THETA, ESTIMATED ERROR IN
C        TWO THETA, WAVE LENGTH
C      STOPPER CARD, FORMAT(14A5,I2), +1 IN COL. 71-72
C      EXTRAPOLATION FUNCTIONS
C      1. DELTA THETA=K1*SINF(2.0*THETA)
C      2. DELTA THETA=K2*COSF(THETA)
C      3. NELSON-RILEY, DELTA THETA=K3*COSF(THETA)*(0.5+SINF(THETA)/(2.0*
C         THETA))
C      4. DELTA THETA=K4
C
      DIMENSION TITLE(14), ALAT(10),ISEL(10), XH(3,500), THETA(500),
     1  ERROR(500), ROW(10),  DC(3,3,6), ALINC(6), ALDEL(6), DP(10),
     2  ANORM(65), AVEC(10), WAVE(500), CORR(10),SDEV(10), ALOUT(10)
   99 READ 101, (TITLE(I), I=1,14), KEY
  101 FORMAT (14A5,I2)
      IF (KEY)  98, 100, 98
  100 PRINT 102, (TITLE(I), I=1,14)
  102 FORMAT (1HC14A5)
      READ 103,  (ALAT(I), I=1,6)
  103 FORMAT (6F10.4)
      PRINT 104, (ALAT(I), I=1,6)
  104 FORMAT (1H030H  INITIAL LATTICE CONSTANTS
     1        /1H02HA=F8.4,4H  B=F8.4,4H  C=F8.4,
     2           8H  ALPHA=F6.2,7H  BETA=F6.2,8H  GAMMA=F6.2)
      READ 105, (ISEL(I),I=1,10), LCODE, NC, DPM, DPA, DPK, NDATA
  105 FORMAT (10I1,2I10,3F10.2,I10)
      PRINT 106, (ISEL(I), I=1,10), NC, DPM, DPA, DPK, NDATA
  106 FORMAT (1HO 8HISEL(I)=10I1,5H  NC=I2,6H  DPM=F4.2,
     1           6H  DPA=F4.2,6H  DPK=F4.2,8H  NDATA=I4)
      GO TO (126,132,123,129,128,130,121),LCODE
  121 PRINT 115
  115 FORMAT (1HC15H  CUBIC LATTICE)
      GO TO 135
  128 PRINT 116
  116 FORMAT (1HC25H  RHOMBOHEDRAL LATTICE    )
      GO TO 135
  129 PRINT 117
```

```
  117 FORMAT (1HC20H  TETRAGONAL LATTICE)
      GO TO 135
  130 PRINT 118
  118 FORMAT (1HC20H  HEXAGONAL LATTICE )
      GO TO 135
  123 PRINT 119
  119 FORMAT (1HC25H  ORTHORHOMBIC LATTICE    )
      GO TO 135
  132 PRINT 120
  120 FORMAT (1HC20H  MONOCLINIC LATTICE)
      GO TO 135
  126 PRINT 134
  134 FORMAT (1HC20H  TRICLINIC LATTICE )
  135 CONTINUE
      READ 107, ((XH(J,I),J=1,3),THETA(I),ERROR(I), WAVE(I), I=1, NDATA)
  107 FORMAT (6F10.0)
      DO 108 I=7, 10
  108 ALAT(I)=0.0
      NV=0
      DO 111 I=1, 10
  111 NV=NV+ISEL(I)
      NP=NV*(NV+3)/2
      NAN=NV+1
      DO 113 I=1, 3
      ALDEL(I)=0.005
      ALAT(I+3)=ALAT(I+3)/57.295800
  113 ALDEL(I+3)=0.5/57.295800
      IC=1
C     START REFINEMENT CYCLES
  176 IF (IC-NC) 1176, 1176, 97
 1176 DO 109 I=1, 10
  109 AVEC(I)=0.0
      DO 110 I=1, NP
  110 ANORM(I)=0.0
      RSUM=0.0
C     OBTAIN DC MATRIX, UPPER TRIANGULAR PORTION, DOUBLED OFF-DIAGONALS
      DO 136 I=1, 3
      DO 136 J=I, 3
      CIJO=CIJ(I,J,ALAT)
      DO 136 K=1, 6
      DC(I,J,K)=0.0
      DO 137 L=1, 6
  137 ALINC(L)=ALAT(L)
      IF (ISEL(K)) 136, 136, 206
  206 ALINC(K)=ALAT(K)+ALDEL(K)
C     SET SYMMETRY RELATED PARAMETERS
      GO TO (201,201,201,202,203,202,205), LCODE
  202 ALINC(2)=ALINC(1)
      GO TO 201
  203 ALINC(5)=ALINC(4)
      ALINC(6)=ALINC(4)
  205 ALINC(3)=ALINC(1)
      GO TO 202
  201 DC(I,J,K)=(CIJ(I,J,ALINC)-CIJO)/ALDEL(K)
  136 CONTINUE
C     START LOOP THROUGH REFLECTION DATA
      DO 141 M=1, NDATA
      DELTA=0.0
      DO 143 I=1, 3
      DO 143 J=I, 3
  143 DELTA=DELTA+CIJ(I,J,ALAT)*XH(I,M)*XH(J,M)
C     CALCULATE DERIVATIVES OF DELTA WITH RESPECT TO LATTICE PARAMETERS
```

```
      DO 142 K=1, 6
      DP(K)=0.0
      DO 142 I=1, 3
      DO 142 J=I, 3
  142 DP(K)=DP(K)+DC(I,J,K)*XH(I,M)*XH(J,M)
      WTHE=THETA(M)/114.59160
      WS2TH=SINF(2.0*WTHE)
      WSTH=SINF(WTHE)
      WCTH=COSF(WTHE)
      WWAV2=WAVE(M)*WAVE(M)
      FLAMB=4.0/WWAV2
      WDELTH= ALAT(7)*WS2TH+ ALAT(8)*WCTH      + ALAT(9)*WCTH*
     1  (0.5+WSTH/(2.0*WTHE))+ALAT(10)
      DELTA=DELTA-FLAMB*(WSTH*WSTH+WDELTH*WS2TH)
      DP(7)=-WS2TH*WS2TH*FLAMB
      DP(8)=-WS2TH*WCTH*FLAMB
      DP(9)=-WS2TH*WCTH*(0.5+WSTH/(2.0*WTHE))*FLAMB
      DP(10)=-WS2TH*FLAMB
      WATE=WWAV2/(ERROR(M)*WS2TH)
      DO 144 I=1, 10
  144 DP(I)=DP(I)*WATE
      DELTA=DELTA*WATE
C     ADD TERMS TO MATRIX
      RSUM=RSUM+DELTA*DELTA
      KK=NV
      K=0
      DO 145 I=1, 10
      IF (ISEL(I)) 145, 145, 146
  146 DO 147 J=I, 10
      IF (ISEL(J)) 147, 147, 148
  148 KK=KK+1
      ANORM(KK)=ANORM(KK)+DP(I)*DP(J)
  147 CONTINUE
      K=K+1
      AVEC(K)=AVEC(K)-DELTA*DP(I)
  145 CONTINUE
  141 CONTINUE
      CALL SYMLIN(ANORM,NV,AVEC,NG)
      IF (NG) 152, 151, 152
  152 PRINT 150
  150 FORMAT (1H035H  NORMAL EQUATIONS ARE SINGULAR     )
      GO TO 99
  151 W=RSUM/(FLOATF(NDATA)-FLOATF(NV))
      DO 161 I=NAN, NP
  161 ANORM(I)=ANORM(I)*W
      DO 153 I=1, 10
      IF (ISEL(I)) 154, 154, 153
  154 CORR(I)=0.0
      SDEV(I)=0.0
  153 CONTINUE
      K=0
      DO 155  I=1, 3
      IF (ISEL(I)) 155, 155, 156
  156 K=K+1
      ALAT(I)=ALAT(I)+ANORM(K)*DPM
      CORR(I)=ANORM(K)*DPM
      KK=K*NV+K-K*(K-1)/2
      SDEV(I)=SQRTF(ANORM(KK))
  155 ALOUT(I)=ALAT(I)
      DO 157 I=4, 6
      IF(ISEL(I)) 157, 157, 158
  158 K=K+1
```

```
      CORR(I)=ANORM(K)*DPA*57.295800
      ALAT(I)=ALAT(I)+ANORM(K)*DPA
      KK=K*(NV+1)-K*(K-1)/2
      SDEV(I)=57.295800*SQRTF(ANORM(KK))
  157 ALOUT(I)=ALAT(I)*57.295800
      DO 159 I=7, 10
      IF (ISEL(I))  159, 159, 160
  160 K=K+1
      CORR(I)=ANORM(K)*DPK*57.295800
      ALAT(I)=ALAT(I)+ANORM(K)*DPK
      KK=K*(NV+1)-K*(K-1)/2
      SDEV(I)=57.295800*SQRTF(ANORM(KK))
  159 ALOUT(I)=ALAT(I)*57.295800
C     SET SYMMETRY RELATED PARAMETERS
      GO TO (1201,1201,1201,1202,1203,1202,1205), LCODE
 1202 ALAT(2)=ALAT(1)
      ALOUT(2)=ALOUT(1)
      GO TO 1201
 1203 ALAT(5)=ALAT(4)
      ALOUT(5)=ALOUT(4)
      ALAT(6)=ALAT(4)
      ALOUT(6)=ALOUT(4)
 1205 ALAT(3)=ALAT(1)
      ALOUT(3)=ALOUT(1)
      GO TO 1202
 1201 CONTINUE
C     OUTPUT RESULTS FOR CYCLE IN ANGSTROMS AND DEGREES
      PRINT 166, IC
  166 FORMAT (1HC 5HCYCLEI3,  32H        A          B          C
     1            40H      ALPHA       BETA      GAMMA    K(1)
     2            39H  K(2)    K(3)    K(4)  RSUM/(NDATA-NV))
      PRINT 170,  (CORR(I), I=1, 10)
  170 FORMAT (1HC10HCHANGE    3F10.4,3F10.3,4F08.4)
      PRINT 171, (ALOUT(I), I=1, 10), H
  171 FORMAT (1HC10HNEW VALUE 3F10.4,3F10.3,4F08.4,E15.5)
      PRINT 172, (SDEV(I), I=1, 10)
  172 FORMAT (1HO10HESD       3F10.4,3F10.3,4F08.4)
C     TEST FOR END OF REFINEMENT
      K=0
      DO 501 I=1, 10
      IF (ISEL(I)) 501, 501, 502
  502 K=K+1
      KK=K*(NV+1)-K*(K-1)/2
      IF ((ABSF(ANORM(K))/SQRTF(ANORM(KK)))-0.1) 501, 503, 503
  501 CONTINUE
      GO TO 97
  503 IC=IC+1
      GO TO 176
C     TERMINATE REFINEMENT
   97 IF (NC) 1401, 1401, 1197
 1197 PRINT 301, (ANORM(I), I=NAN, NP)
  301 FORMAT(1HO 50H  VARIANCE-COVARIANCE MATRIX IN ANGSTROMS AND RADI
     1            5HANS  /(1H07E15.6))
      DO 302 K=1, NV
      KK=K*(NV+1)-K*(K-1)/2
  302 SDEV(K)=1.0/SQRTF(ANORM(KK))
      PRINT 303
  303 FORMAT(1HO 20H  CORRELATION MATRIX)
      KK=NAN
      DO 304 I=1, NV
      DO 305 J=1, NV
  305 ROW(J)=0.0
```

```
      DO 306 J=I, NV
      ROW(J)=ANORM(KK)*SDEV(I)*SDEV(J)
  306 KK=KK+1
      PRINT 307, (ROW(J), J=1, NV)
  307 FORMAT(1HO 10F10.4)
  304 CONTINUE
C     OUTPUT REFLECTION DATA
 1401 PRINT 401
  401 FORMAT(1HO 45H                                          OBSERVED
     1           45H     ESTIMATED       CALCULATED      CALCULATED /1H
     2           45H          H          K          L     TWO THETA
     3           45H      ERROR           TWO THETA           DRIFT
     4           15H       LAMBDA    )
      DO 402 M=1, NDATA
      DELTA=0.0
      DO 403 I=1, 3
      DO 403 J=I, 3
  403 DELTA=DELTA+CIJ(I,J,ALAT)*XH(I,M)*XH(J,M)
      WTHE=THETA(M)/114.59160
      WS2TH=SINF(2.0*WTHE)
      WSTH=SINF(WTHE)
      WCTH=COSF(WTHE)
      WWAV2=WAVE(M)*WAVE(M)
      WDELTH=ALAT(7)*WS2TH+ALAT(8)*WCTH+ALAT(9)*WCTH*
     1  (0.5+WSTH/(2.0*WTHE))+ALAT(10)
      CALC=114.59160*ASINF(SQRTF(WWAV2*DELTA/4.0-WDELTH*WS2TH))
      DRIFT=114.59160*WDELTH
      PRINT 404, (XH(I,M),I=1,3), THETA(M), ERROR(M),CALC,DRIFT,WAVE(M)
  404 FORMAT(1HO 3F10.0, F12.2, 3F15.2, F15.6)
  402 CONTINUE
      GO TO 99
   98 STOP 87
      END


     END       ACCNTA0015  @D.WILLIAMS@                                    POGO
     START     ACCNTA0015  @D.WILLIAMS@                                    PUGO
     COMPILE   RUN  FORTRAN LIST                                           PUGO
C     FUNCTION CIJ(I,J,ALAT), J IS EQUAL OR GREATER THAN I
      FUNCTION CIJ(I,J,ALAT)
      DIMENSION ALAT(6)
      COSA=COSF(ALAT(4))
      COSB=COSF(ALAT(5))
      COSC=COSF(ALAT(6))
      DET=1.0/(1.0-COSA*COSA-COSB*COSB-COSC*COSC+2.0*COSA*COSB*COSC)
      GO TO (7,8,6), I
    7 GO TO (1,2,3), J
    8 GO TO (9,4,5), J
    1 CIJ=DET*(1.0-COSA*COSA)/(ALAT(1)*ALAT(1))
      GO TO 9
    2 CIJ=DET*(COSA*COSB-COSC)*2.0/(ALAT(1)*ALAT(2))
      GO TO 9
    3 CIJ=DET*(COSA*COSC-COSB)*2.0/(ALAT(1)*ALAT(3))
      GO TO 9
    4 CIJ=DET*(1.0-COSB*COSB)/(ALAT(2)*ALAT(2))
      GO TO 9
    5 CIJ=DET*(COSB*COSC-COSA)*2.0/(ALAT(2)*ALAT(3))
      GO TO 9
    6 CIJ=DET*(1.0-COSC*COSC)/(ALAT(3)*ALAT(3))
    9 RETURN
      END
```

```
      END        ACCNTA0015  @D.WILLIAMS@                                  PCGC
      START      ACCNTA0015  @D.WILLIAMS@                                  PCGC
      COMPILE    RUN  FORTRAN LIST                                         PCGC
C      SYMMETRIC LINEAR EQUATION SOLVER USING SYMINV
       SUBROUTINE SYMLIN(AM, NV, VEC, ISING)
       DIMENSION AM(9869), VEC(139)
       CALL SYMINV (AM, NV, ISING)
       IF (ISING) 99, 2, 99
     2 DO 3 I=1, NV
       AM(I)=0.0
       DO 3 J=1, NV
       IF (J-I) 4, 5, 5
     5 IJMUL=I*NV+J-(I*(I-1))/2
       GO TO 6
     4 IJMUL=J*NV+I-(J*(J-1))/2
     6 AM(I)=AM(I)+AM(IJMUL)*VEC(J)
     3 CONTINUE
    99 RETURN
       END


      END        ACCNTA0015  @D.WILLIAMS@                                  PCGC
      START      ACCNTA0015  @D.WILLIAMS@                                  PCGC
      COMPILE    RUN  FORTRAN LIST                                         PCGC
C      INVERT POSITIVE DEFINITE SYMMETRIC MATRIX OF ORDER NV  D.WILLIAMS
C      MATRIX IS STORED AS FOLLOWS
C      N STORAGE CELLS TO BE USED AS WORK CELLS BY INVERTER, FOLLOWED BY
C      MATRIX ELEMENTS BY ROWS, GIVING ONLY UPPER TRIANGULAR PART
C      A TOTAL OF  NV*(NV+3)/2 STORAGE CELLS IS REQUIRED
C      LOCATION AM(NV+1) IS STARTING ADDRESS OF MATRIX
C      NG=0 IS NORMAL RETURN, NG=1 IS RETURN FOR SINGULAR MATRIX
C      INVERSE MATRIX IS RETURNED TO SAME LOCATION I.E. AM(NV+1)
C      METHOD-BUSING AND LEVY, COMM. ACM, AUGUST 1962
       SUBROUTINE SYMINV(AM, NV, NG)
       DIMENSION AM(9869)
C      DIAGONALIZE
       DO 24 I=1, NV
       IO=I*NV-(I*(I-1))/2
       II=IO+I
       LI=(I-1)*NV+I-((I-1)*(I-2))/2
       AM(LI)=FLOATF(I)
       BIGAJJ=0.0
       DO 2  J=I, NV
       JJ=J*NV+J-(J*(J-1))/2
       IF (ABSF(AM(JJ))-BIGAJJ)  2, 2, 3
     3 BIGAJJ=ABSF(AM(JJ))
       AM(LI)=FLOATF(J)
     2 CONTINUE
       CALL AINTCH(AM,NV,I,IO,II,LI)
C      RESUME DIAGONALIZE
    20 IF(AM(II)) 22, 22, 21
    22 NG=1
       GO TO 62
    21 AM(II)=1.0/AM(II)
       IQO=(I-1)*NV-((I-1)*(I-2))/2
       I1=I+1
       IF(I1-NV)  28, 28, 29
    28 DO 23 K=I1, NV
       IK=IO+K
       IKQ=IQO+K
```

```
   23 AM(IKQ)=-AM(II)*AM(IK)
      DO 24 J=I1, NV
      JO=J*NV-(J*(J-1))/2
      IJ=IO+J
      DO 24 K=J, NV
      JK=JO+K
      IKQ=IQO+K
   24 AM(JK)=AM(JK)+AM(IKQ)*AM(IJ)
C     RESTORE
   29 I=NV-1
   55 IO=I*NV-(I*(I-1))/2
      II=IO+I
      LI=(I-1)*NV+I-((I-1)*(I-2))/2
      I1=I+1
      DO 50 J=I1, NV
      IJ=IO+J
   50 AM(IJ)=0.0
      IQO=(I-1)*NV-((I-1)*(I-2))/2
      DO 52 J=I1, NV
      JO=J*NV-(J*(J-1))/2
      IJ=IO+J
      IJQ=IQO+J
      DO 30  K=J, NV
      IK=IO+K
      JK=JO+K
      AM(IK)=AM(IK)+AM(IJQ)*AM(JK)
      IF (J-K)  53, 30, 53
   53 IKQ=IQO+K
      AM(IJ)=AM(IJ)+AM(IKQ)*AM(JK)
   30 CONTINUE
   52 AM(II)=AM(II)+AM(IJQ)*AM(IJ)
C     INTERCHANGE
      CALL AINTCH(AM,NV,I,IO,II,LI)
      I=I-1
      IF (I) 61, 61, 55
   61 NG=0
   62 RETURN
      END


     END        ACCNTA0015  @D.WILLIAMS@                                    POGO
     START      ACCNTA0015  @D.WILLIAMS@                                    POGO
     COMPILE    RUN  FORTRAN LIST                                           POGO
C     INTERCHANGE SUBROUTINE FOR SYMINV      D.WILLIAMS
      SUBROUTINE AINTCH(AM,NV,I,IO,II,LI)
      DIMENSION AM(9869)
   10 LI=XINTF(AM(LI))
      IF(LI-I) 15, 16, 15
   15 ILI=IO+LI
      LIO=LI*NV-(LI*(LI-1))/2
      DO 11 J=I, NV
      IJ=IO+J
      WORK=AM(IJ)
      IF(LI-J) 13, 13, 12
   12 JLI=J*NV+LI-(J*(J-1))/2
      AM(IJ)=AM(JLI)
      AM(JLI)=WORK
      GO TO 11
   13 LIJ=LIO+J
      AM(IJ)=AM(LIJ)
      AM(LIJ)=WORK
   11 CONTINUE
```

```
   WORK=AM(II)
   AM(II)=AM(ILI)
   AM(ILI)=WORK
16 RETURN
   END

  END        ACCNTA0015  @D.WILLIAMS@                                  PUGO
```